Models to Estimate Physical/Chemical Properties of Chemicals

The PHYSICAL/CHEMICAL PROPERTY MODELS included in this section are:

- ❖MPBPVP™
- ❖WSKOWWIN™
- ❖KOWWIN™
- ❖HENRYWIN™
- ❖WVOLWIN™
- ❖PCKOCWIN™

Following are brief fact sheets providing information on the models OPPT has developed and uses to estimate environmental fate of chemicals. Information provided on each model includes:

- ❖What physical/chemical property does the model estimate?
- ❖What is significant about the physical/chemical property to risk assessment?
- ❖Why is knowing physical/chemical properties important?
- ❖Why would I want to use the model?
- ❖What do I need to run the model?
- ❖What are the inputs and outputs for the model?

MPBPVP™ to Estimate Melting Point, Boiling Point, and Vapor Pressure

What Does the MPBPVP™ Model Do?

MPBPVP™ estimates an organic chemical's melting point, boiling point, and vapor pressure at 25 deg C using a combination of techniques.

How are the model predictions useful in risk assessment?

Melting Point (MP), the temperature at which a chemical changes from solid to liquid, gives clues to other chemical properties:
❖MP indicates the state (solid-liquid-gas) of the chemical in the ambient environment.
❖High MP indicates low water solubility.
❖Low MP indicates increased absorption is possible through the skin, GI tract, or lungs.
❖The range of measured MPs indicates it purity: narrow = more pure, wide = less pure.
❖MP <100^{O}C = increased volatility and higher potential exposures.

Boiling Point (BP), the temperature at which the VP of a chemical in a liquid state equals atmospheric pressure, gives clues to other chemical properties:
❖High BP indicates low VP, for example structurally large substances like polymers.

Vapor Pressure (VP), the pressure at which a liquid and its vapor are in equilibrium at a given temperature, gives clues to other chemical properties:
❖Chemicals with VP $\geq 10^{-4}$ mm Hg (higher VP) exist mostly in the vapor phase in the atmosphere, and often have higher potential inhalation exposures than chemicals with low vapor pressure.
❖Chemicals with VP 10^{-5} to 10^{-7} mm Hg exist in both vapor and solids or particulate phases.
❖Chemicals with (lower VP) $\leq 10^{-8}$ mm Hg exist mostly as solids.

Inputs Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a “Batch Mode” so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

❖Molecular weight and formula
❖Estimations of melting point, boiling point, and vapor pressure at 25 deg C
❖Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Examples of Melting Point, Boiling Point, and Vapor Pressure Values

Examples of Melting Points at 25 deg C

CAS RN	Chemical	Degrees C
60571	Dieldrin	135
108952	Phenol	-2
75092	Dichloromethane	-90
67641	Acetone	-94
50000	Formaldehyde	-111

Examples of Boiling Points at 25 deg C

CAS RN	Chemical	Degrees C
60571	Dieldrin	340
108952	Phenol	170
75092	Dichloromethane	80
67641	Acetone	45
50000	Formaldehyde	10

Examples of Vapor Pressures at 25 deg C

CAS RN	Chemical	Degrees C
60571	Dieldrin	1.77E-5
108952	Phenol	1
75092	Dichloromethane	86
67561	Methanol	396
50000	Formaldehyde	1330

Sample Output from the MPBPVP™ Model

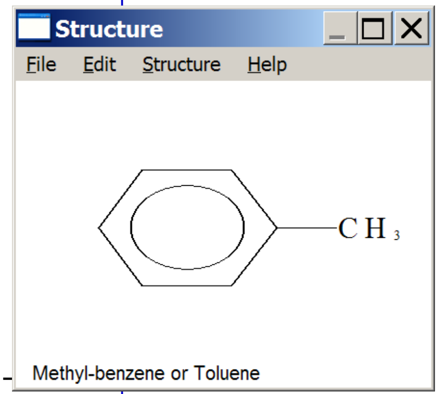
Where Can I Get MPBPVP™?

MPBPVP™ v1.40 has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run MPBPVP™ as a stand-alone model by putting a shortcut to the MPBPWIN.exe file on your Windows Desktop.

Saving Output

Results can be printed when displayed. After results are displayed click on “Save Results” and you can save results as a “.dat” file that can be opened using MSWord or WordPerfect. Output can also be copied (click on “Copy”) through the Windows Clipboard. Structures can be saved as an ISIS “.skc” file or through the Windows Clipboard. Further explanations are given in “Help” on the Results page.

INPUTS: CAS Number 108883 (Methyl-benzene or toluene)



RESULTS:

```
Experimental Database Structure Match:
  Name      :  TOLUENE
  CAS Num   :  000108-88-3
  Exp MP (deg C):   -94.9
  Exp BP (deg C):   110.6
  Exp VP (mm Hg):   2.84E+01
  Exp VP (deg C):   25
  Exp VP ref     :  DAUBERT,TE & DANNER,RP (1985)

SMILES : c(cccc1)(c1)C
CHEM   : Methyl-benzene or Toluene
MOL FOR: C7 H8
MOL WT : 92.14
------------------- SUMMARY MPBPWIN v1.40 -----------

Boiling Point:  125.72 deg C (Adapted Stein and Brown
Method)

Melting Point:  -78.09 deg C (Adapted Joback Method)
Melting Point:  -40.26 deg C (Gold and Ogle Method)
Mean Melt Pt :  -59.17 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  -59.17 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
   (Using BP: 110.60 deg C (exp database))
   (MP not used for liquids)
     VP:  25.1 mm Hg (Antoine Method)
     VP:  22.3 mm Hg (Modified Grain Method)
     VP:  29.2 mm Hg (Mackay Method)
  Selected VP:  23.7 mm Hg (Mean of Antoine & Grain methods)
-------+-----+--------------------+----------+---------
 TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   21.98  |   21.98
 Group |  5  |  CH (aromatic)     |   28.53  |  142.65
 Group |  1  |  -C (aromatic)     |   30.76  |   30.76
   *   |     |  Equation Constant |          |  198.18
=============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  393.57
RESULT- corr |  BOILING POINT in deg Kelvin  |  398.88
             |  BOILING POINT in deg C       |  125.72
-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  |  -CH3              |   -5.10  |   -5.10
 Group |  5  |  CH (aromatic)     |    8.13  |   40.65
 Group |  1  |  -C (aromatic)     |   37.02  |   37.02
   *   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin  |  195.07
             |  MELTING POINT in deg C       |  -78.09
-------------------------------------------------------
```

Melting point is calculated by two different methods, the mean value is determined, and the mean is selected as the melting point.

Vapor pressure is also calculated by different methods, and the mean value is selected as the vapor pressure.

WSKOWWIN™ to Estimate Water Solubility

What Does the WSKOWWIN™ Model Do?

WSKOWWIN™ estimates an octanol-water partition coefficient using the algorithms in the KOWWIN program and estimates a chemical's water solubility from this value. This method uses correction factors to modify the water solubility estimate based on regression against log Kow. This model can tell an assessor if the compound will dissolve in surface water. Water solubility is the degree to which a compound will dissolve in water. It is reported as the amount of the chemical (in milligrams) that will dissolve in 1 liter of water (mg/L).

How are the model predictions useful in risk assessment?

Knowing a chemicals water solubility (WS) is important because this can tell an assessor important information about the chemical's potential risk, for example:

- Chemicals with low WS:
  - Will have low concentration in aqueous media
  - Have a higher fish BCF
  - Are less likely to be absorbed into mammalian tissues.
- Chemicals with high WS:
  - Are more likely to be transported along with the water during storm events or to ground water; and
  - Have low log KOW values, and are more likely to be absorbed through GI tract, or lungs. The exception is the case of dispersible molecules like surfactants, and detergents, which can have high predicted log KOWs and can be absorbed through the lung.

Inputs: Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs:

- Molecular weight and formula
- Water solubility at 25°C (milligrams per liter)
- Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Examples of Water Solubility Values

Solubility Classification (mg/L or ppm):

Very soluble	> 10,000
Soluble	> 1,000 - 10,000
Moderately sol.	> 100 - 1,000
Slightly soluble	> 0.1 - 100
Insoluble	< 0.1

Water Solubility Classifications

CAS No.	Chemical	Water Sol. (mg/L)
67561	Methanol	1.00E+06
67641	Acetone	2.20E+05
50000	Formaldehyde	5.74E+04
1912249	Atrazine	2.14E+02
60571	Dieldrin	1.46E-01

Important Notes

WSKOWWIN is not appropriate for dispersible compounds, including surfactants.

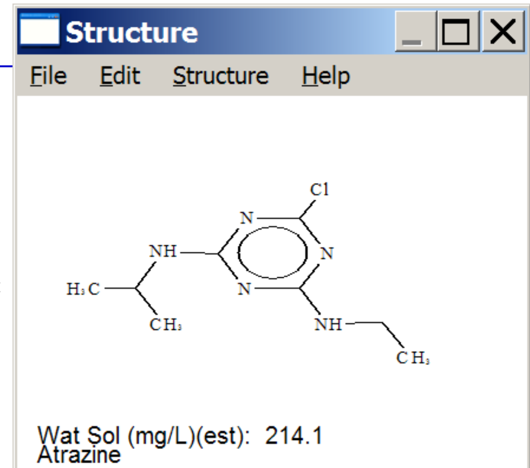
Where Can I Get WSKOWWIN™?

WSKOWWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm If you download and install EPI Suite™ you can run WSKOWWIN™ as a stand-alone model by putting a shortcut to the WSKOWNT.exe file on your Windows Desktop.

WSKOWWIN™ to Estimate Water Solubility

Saving Output

Results can be printed when displayed. After results are displayed click on “Save Results” and you can save results as a “.dat” file that can be opened using MSWord or WordPerfect. Output can also be copied (click on “Copy”) through the Windows Clipboard. Structures can be saved as an ISIS “.skc” file or through the Windows Clipboard. Further explanations are given in “Help” on the Results page.



INPUTS: CAS Number 1912249 (atrazine)

RESULTS:

```
Water Sol: 214.1 mg/L

Experimental Water Solubility Database Match:
   Name      :  ATRAZINE
   CAS Num   :  001912-24-9
   Exp WSol  :  34.7 mg/L (26 deg C)
   Exp Ref   :  WARD,TM & WEBER,JB (1968)

SMILES : n(c(nc(n1)NC(C)C)NCC)c1CL
CHEM   : Atrazine
MOL FOR: C8 H14 CL1 N5
MOL WT : 215.69
------------------------- WSKOW v1.40 Results -------------------
Log Kow  (estimated)   :  2.82
Log Kow (experimental):  2.61
    Cas No: 001912-24-9
    Name  : Atrazine
    Refer : Hansch,C et al. (1995)
Log Kow used by Water solubility estimates:  2.61

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -3.003
   Water Solubility at 25 deg C (mg/L):  214.1
```

KOWWIN™ to Estimate Octanol-Water Partition Coefficient (KOW)

What Does the KOWWIN™ Model Do?

KOWWIN estimates the log octanol-water partition coefficient, log Kow, of chemicals using an atom/fragment contribution method.

How are the model predictions useful in risk assessment?

Knowing KOW will help the risk assessor know where the chemical will go in the stream. KOW indicates whether a chemical predominantly will be found in water (is hydrophilic) or in fatty tissue of animals or other organic materials (is lipophilic) in an aquatic environment. Lipophilic chemicals can bioaccumulate in fatty tissue of fish and bioconcentrate in animals (including humans) that consume the fish. Chemicals with a log KOW in the range of 4-7 may bioconcentrate significantly.

Inputs

Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

❖Log KOW
❖Molecular weight and formula
❖Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Examples of KOW Values

	CAS Number	Chemical	log KOW
lipophilic	25051243	deca-PCB	10.2
	50293	DDT	6.8
	60571	Dieldrin	5.2
	1912249	Atrazine	2.6
	50000	Formaldehyde	0.4
hydrophilic	67641	Acetone	-0.2

log KOW of 0 indicates an equal affinity for lipids and for water

Important Notes

❖KOW is often reported as a **log** due to the extremely wide range of measured KOW values.
❖A log KOW of 0 indicates an equal affinity for lipids and for water.
❖**There is a unique relationship between Log KOW and BCF:** As log KOW increases the solubility in lipids increases. This means an increase in the potential to bioconcentrate in organisms. This relationship begins to change around log KOW of 6. For chemicals with log KOW exceeding 6 the potential to bioconcentrate begins to drop approaching 0 at log KOW of 12.

Where Can I Get KOWWIN™?

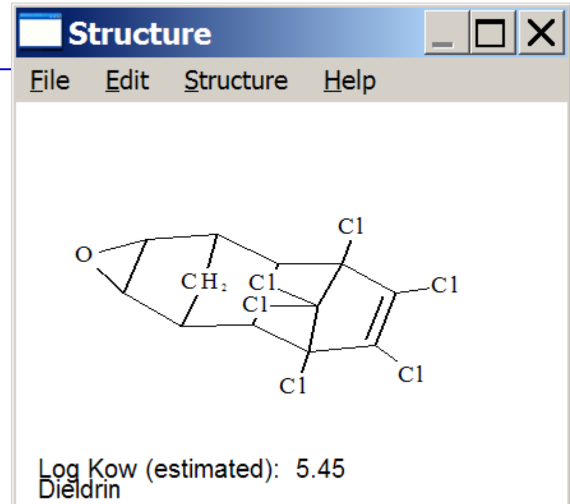
KOWWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run KOWWIN ™ as a stand-alone model by putting a shortcut to the KOWWINNT.exe file on your Windows Desktop.

Saving Output

Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

KOWWIN™ to Estimate Octanol-Water Partition Coefficient (KOW)

Sample Output from the KOWWIN™ Model



INPUTS: CAS Number 60571 (dieldrin)

RESULTS:

Log Kow (version 1.66 estimate): 5.45

```
Experimental Database Structure Match:
   Name       :  Dieldrin
   CAS Num    :  000060-57-1
   Exp Log P:  5.40
   Exp Ref    :  DeBruijn,J et al. (1989)

Experimental Database Structure Match:
   Name       :  Endrin
   CAS Num    :  000072-20-8
   Exp Log P:  5.20
   Exp Ref    :  DeBruijn,J et al. (1989)

SMILES : CLC4=C(CL)C5(CL)C3C1CC(C2OC12)C3C4(CL)C5(CL)CL
CHEM    : Dieldrin
MOL FOR: C12 H8 CL6 O1
MOL WT : 380.91
```

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	6	-CH [aliphatic carbon]	0.3614	2.1684
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	2	=CH- or =C< [olefinc carbon]	0.3836	0.7672
Frag	1	-O- [oxygen, aliphatic attach]	-1.2566	-1.2566
Frag	4	-CL [chlorine, aliphatic attach]	0.3102	1.2408
Frag	2	-CL [chlorine, olefinic attach]	0.4923	0.9846
Frag	2	-tert Carbon [3 or more carbon attach]	0.2676	0.5352
Factor	2	Fused aliphatic ring unit correction	-0.3421	-0.6842
Const		Equation Constant		0.2290

Log Kow = 5.4478

HENRYWIN™ to Estimate Henry's Law Constant

What Does the HENRYWIN™ Model Do?

HENRYWIN™ estimates the Henry's Law Constant (HLC) of an organic compound by two different methods. It also can estimate the HLC of an unknown compound based on the HLC of a known compound. The ratio of the vapor pressure to the water solubility is an estimate of the HLC that is sufficient for most purposes. HLC gives a relative measure of the volatility of a compound from water by measuring the extent to which a compound will partition between water and the air.

How are the model predictions useful in risk assessment?

Knowing the HLC helps the risk assessor predict the fate of the chemical once it is released to surface water. High HLC indicates chemical is likely to volatilize from solution and partition in air. Low HLC indicates chemical is not likely to volatilize and will remain in surface water.

Note: This estimate of the HLC does not apply for very water-soluble (I.e. miscible) compounds.

Inputs

Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

- ❖Molecular weight and formula
- ❖Henry's Law Constant estimated by bond contribution method and by group contribution method (best used for pesticides)
- ❖Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Examples of Henry's Law Constant Values

CAS Number	Chemical	HLC (atm-m^3/mole)
75092	Dichloromethane	3.0E-03
50000	Formaldehyde	6.1E-05
67641	Acetone	4.0E-05
67561	Methanol	4.4E-06
60571	Dieldrin	5.4E-07

Volatility Classifications

Very volatile	$\geq 10^{-1}$
Volatile	10^{-1} - 10^{-3}
Moderately volatile	10^{-3} - 10^{-5}
Slightly volatile	10^{-5} - 10^{-7}
Nonvolatile	$< 10^{-7}$

Where Can I Get HENRYWIN™?

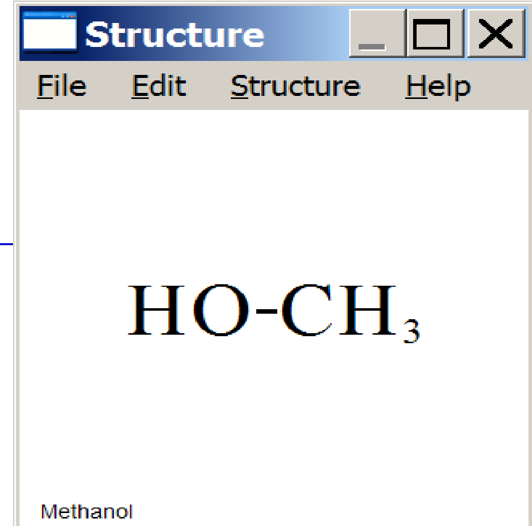
HENRYWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run HENRYWIN™ as a stand-alone model by putting a shortcut to the HENRYNT.exe file on your Windows Desktop.

Saving Output

Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

HENRYWIN™ to Estimate Henry's Law Constant

Sample Output From the HENRYWIN™ Model



INPUTS: CAS Number 67561 (methanol)

RESULTS:

```
               Bond Est :  4.27E-006 atm-m3/mole
               Group Est:  3.62E-006 atm-m3/mole
SMILES : OC
CHEM   : Methanol
MOL FOR: C1 H4 O1
MOL WT : 32.04
--------------------------- HENRYWIN v3.10 Results --------------------------

Experimental Database Structure Match:
  Name      :  METHANOL
  CAS Num   :  000067-56-1
  Exp HLC   :  4.55E-06 atm-m3/mole
  Temper    :  25 deg C
  Exp Ref   :  GAFFNEY,JS ET AL. (1987)

----------+----------------------------------------------+---------+----------
   CLASS  |      BOND CONTRIBUTION DESCRIPTION           | COMMENT |  VALUE
----------+----------------------------------------------+---------+----------
 HYDROGEN |  3  Hydrogen to Carbon (aliphatic) Bonds     |         | -0.3590
 HYDROGEN |  1  Hydrogen to Oxygen Bonds                 |         |  3.2318
 FRAGMENT |  1  C-O                                      |         |  1.0855
 FACTOR   |  *  Non-cyclic alkyl or olefinic alcohol     |         |  -.2000
----------+----------------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE    |  TOTAL  |  3.758
----------+----------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 4.27E-006 atm-m3/mole
                                = 1.74E-004 unitless


--------+------------------------------------------------+------------+--------
        |          GROUP CONTRIBUTION DESCRIPTION        |   COMMENT  |  VALUE
--------+------------------------------------------------+------------+--------
        |            1   CH3 (X)                         |            | -0.62
        |            1   O-H (C)                         |            |  4.45
--------+------------------------------------------------+------------+--------
 RESULT |   GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |    TOTAL   |  3.83
--------+------------------------------------------------+------------+--------
HENRYs LAW CONSTANT at 25 deg C = 3.62E-006 atm-m3/mole
                                = 1.48E-004 unitless
```

Two methods are used to estimate HLC. The group contribution method is best used for pesticides.

PCKOCWIN™ to Estimate Organic Carbon Adsorption Coefficient (KOC)

What Does the PCKOCWIN™ Model Do?

PCKOCWIN™ predicts a chemicals soil adsorption coefficient (KKO), which is the ability of a chemical to sorb to the organic portion of soil and sediment. Koc estimations are based on the Sabljic molecular connectivity method with improved correction factors. KOC is the ratio of amount of chemical adsorbed per unit mass of organic carbon (the "OC") in soils, sediments, or sludge to the concentration of the chemical in the solution at equilibrium. KOC indicates whether a chemical is likely to be be found in water or the organic carbon portion of soils or sediments.

How are the model predictions useful in risk assessment?

KOC provides an indication of partitioning to sediments and sludge. Low KOC values suggest the chemical is likely to remain in water, and possibly migrate with ground water, because it is not likely to sorb to soils, sediments, or sludge. High KOC value suggests the chemical will sorb to soils and sediments, or sludge, and is not likely to be found in surface water or migrate with ground water.

Inputs

Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

- Estimated KOC
- Molecular weight and formula
- Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Examples of KOC Values

CAS Number	Chemical	Log KOC
60571	Dieldrin	4.025
1912249	Atrazine	2.362
75092	Dichloromethane	1.376
106898	Epichlorohydrin	0.652
67641	Acetone	0.297

KOC Classifications

Very strong	$\geq$ 4.5
Strong	3.5 - 4.4
Moderate	2.5 - 3.4
Low	1.5 - 2.4
Negligible	< 1.5

Important Notes

- Like KOW, KOC is also often reported as a log due to the extremely wide range of measured KOC values.
- When Log KOC ≥ 4.5 chemical will largely be removed by sorption to sludge in wastewater treatment plants.

Where Can I Get PCKOCWIN™?

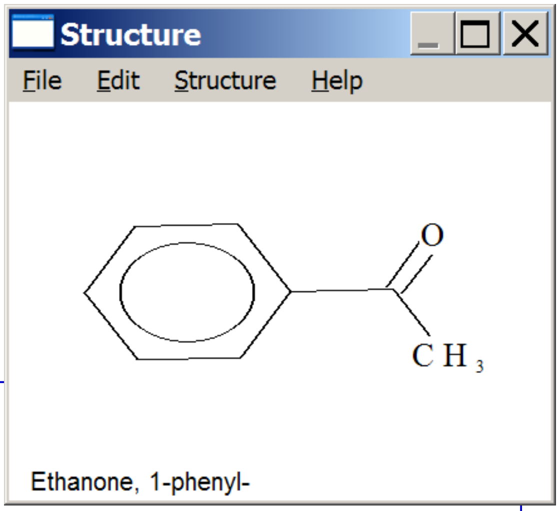
PCKOCWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run PCKOCWIN™ as a stand-alone model by putting a shortcut to the PCKOCNT.exe file on your Windows Desktop.

PCKOCWIN™ to Estimate Organic Carbon Adsorption Coefficient (KOC)

Saving Output

Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

Sample Output From the PCKOCWIN™ Model



INPUTS: CAS Number 98-86-2 (Acetophenone)

RESULTS:

```
Koc (estimated): 46.2

SMILES : O=C(c(cccc1)c1)C
CHEM   : Ethanone, 1-phenyl-
MOL FOR: C8 H8 O1
MOL WT : 120.15
---------------- PCKOCWIN v1.66 Results -------------------

  First Order Molecular Connectivity Index  .... :   4.305
  Non-Corrected Log Koc  ...................... :   2.9123
  Fragment Correction(s):
             1   Ketone  (-C-CO-C-)  .......... : -1.2477
Corrected Log Koc  ........................... :   1.6646

                       Estimated Koc:  46.2
```

Models to Estimate Chemical Fate in the Environment

The ENVIRONMENTAL FATE MODELS included in this section are:

- AOPWIN™
- HYDROWIN™
- BIOWIN™
- BCFWIN™
- STPWIN™
- LEV3EPI™

Following are brief fact sheets providing information on the models OPPT has developed and uses to estimate environmental fate of chemicals. Information provided on each model includes:

- What fate property does the model estimate?
- What is significant about the fate property to risk assessment?
- Why is knowing fate properties important?
- Why would I want to use the model?
- What do I need to run the model?
- What are the inputs and outputs for the model?

AOPWIN™ to Estimate Atmospheric Oxidation Potential

What Does the AOPWIN™ Model Do?

AOPWIN™ estimates rate constants and half-lives of atmospheric reactions of organic compounds released to the air with hydroxyl radicals (-OH) and with ozone in the atmosphere.
estimates the rate at which certain organic compounds will be destroyed by reactions with compounds in the atmosphere.

How are the model predictions useful in risk assessment?

The rate at which an organic compound will be oxidized (destroyed) is an indication of the length of time the compound may reside in the atmosphere.

Inputs

Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

❖Molecular weight and formula
❖Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file
❖Hydroxyl radical (-OH) rate constant and half-life
❖Ozone reaction constant and half-life (for olefins and acetylenes only)

Examples of Atmospheric Oxidation Potential Values

CAS Number	Chemical	AOP 1/2 Life (days)
75092	Dichloromethane	79.3
67641	Acetone	52.4
67561	Methanol	17.4
60571	Dieldrin	1.2
1912249	Atrazine	0.4

Atmospheric Oxidation Potential Classifications

Rapid	$\leq$ 2 hrs
Moderate	2 hrs - $\leq$ 1 day
Slow	> 1 day - $\leq$ 10 days
Negligible	> 10 days

Important Notes

❖Half-life of >2 days indicates the chemical may be persistent in air.
❖If a chemical has a high AOP rate there still is a potential for inhalation exposure if the travel time from source to receptor is greater than the time for complete oxidation of the compound.

Where Can I Get AOPWIN™?

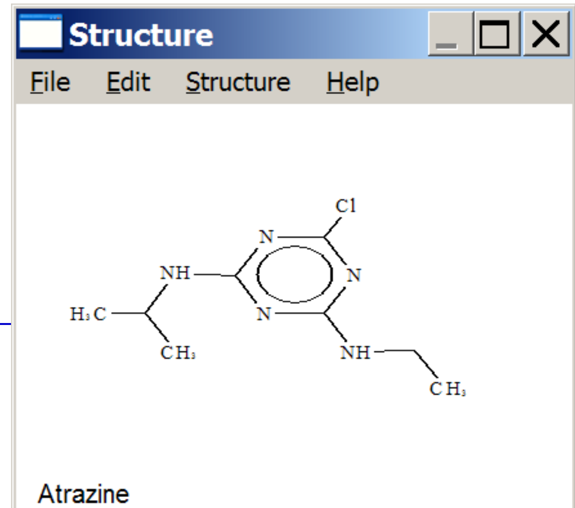
AOPWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run AOPWIN™ as a stand-alone model by putting a shortcut to the AOPWINNT.exe file on your Windows Desktop.

AOPWIN™ to Estimate Atmospheric Oxidation Potential

Saving Output

Results can be printed when displayed. After results are displayed click on “Save Results” and you can save results as a “.dat” file that can be opened using MSWord or WordPerfect. Output can also be copied (click on “Copy”) through the Windows Clipboard. Structures can be saved as an ISIS “.skc” file or through the Windows Clipboard. Further explanations are given in “Help” on the Results page.

Sample Output from the AOPWIN™ Model



INPUTS: CAS Number 1912249 (atrazine)

RESULTS:

```
SMILES  :   n(c(nc(n1)NC(C)C)NCC)c1CL
CHEM    :   Atrazine
MOL FOR :   C8 H14 CL1 N5
MOL WT  :   215.69
-------------------------SUMMARY : HYDROXYL RADICALS-----------------

Hydrogen Abstraction               = 24.2300 E-12 cm3/molecule-sec
Reaction with N, S, and -OH        = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds           = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds         = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings       = 0.1176 E-12 cm3/molecule-sec
Addition to Fused Rings            = 0.0000 E-12 cm3/molecule-sec

     OVERALL OH       =    27.3476 E-12 cm3/molecule-sec
     HALF-LIFE        =    0.391 Days (12-hr day; 1.5E6 OH/cm3)
     HALF-LIFE        =    4.693 Hrs

 . . . . * * Designates Estimation(s) Using ASSUMED Value(s) . . . . . .
-----------------SUMMARY  (AOP v1.90): OZONE REACTION-----------------

     * * * *   NO OZONE REACTION ESTIMATION   * * * *
        (ONLY Olefins and Acetylenes are Estimated)

Experimental Database  :  NO Structure Matches

---------------------------------------------------------------------
```

Reactions with ozone are estimated only for olefins and acetylenes.

HYDROWIN™ to Estimate Hydrolysis

What Does the HYDROWIN™ Model Do?

HYDROWIN™ estimates acid- and base-catalyzed rate constants for chemicals in certain classes (esters, carbamates, epoxides, halomethanes, and certain alkyl halides). A chemical's hydrolytic half-life under typical environmental conditions is also determined. Neutral hydrolysis rates are currently not estimated.

How are the model predictions useful in risk assessment?

Understanding a chemicals rates of hydrolysis (the breakdown of a chemical by its reaction with water) will help the risk assessor estimate the concentration of the compound in treatment systems and after it is released to surface water, and how long the chemical and/or it's hydrolysis products will remain in water bodies after release. The chemical can be catalyzed (broken down) by acids (hydronium) or bases (hydroxide ions).

Inputs

Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

- Molecular weight and formula
- Estimated hydrolysis at 25°C
- Half-life at pHs 8 and 7
- Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Examples of Hydrolysis Values

CAS Number	Chemical	Hydrolysis 1/2 Life (yrs)
51796	Carbamic acid, ethyl ester	3326.534
110383	Ethyl decanonate	7.7

Where Can I Get HYDROWIN™?

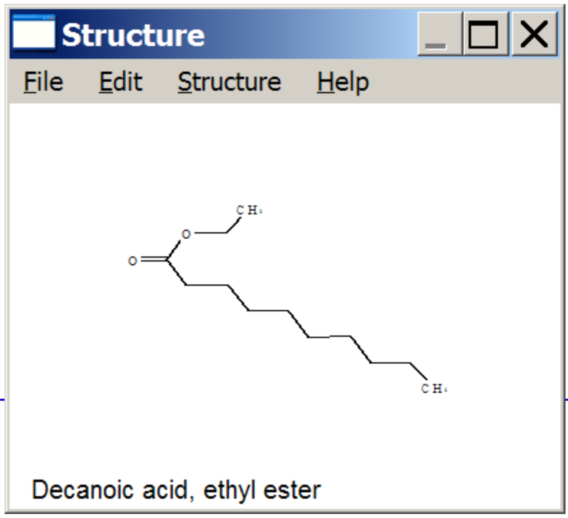
HYDROWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run HYDROWIN™ as a stand-alone model by putting a shortcut to the HYDRONT.exe file on your Windows Desktop.

Saving Output

Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

HYDROWIN™ to Estimate Hydrolysis

Sample Output from the HYDROWIN™ Model



INPUTS: CAS Number 110-38-3
(Ethyl decanonate)

RESULTS:

```
SMILES : O=C(OCC)CCCCCCCCC
CHEM   : Decanoic acid, ethyl ester
MOL FOR: C12 H24 O2
MOL WT : 200.32
---------------------- HYDROWIN v1.67 Results -----------------------

NOTE: Fragment(s) on this compound are NOT available from the
fragment
    library. Substitute(s) have been used!!  Substitute R1, R2, R3,
    or R4 fragments are marked with double asterisks "**".

ESTER:  R1-C(=O)-O-R2                ** R1: n-Octyl-
                                        R2: -CH2-CH3
 Kb hydrolysis at atom #  2:  2.848E-002  L/mol-sec

 Total Kb for pH > 8 at 25 deg C :  2.848E-002  L/mol-sec
 Kb Half-Life at pH 8:     281.632 days
 Kb Half-Life at pH 7:       7.711  years
```

BIOWIN™ to Estimate Biodegradation

What Does the BIOWIN™ Model Do?

BIOWIN provides estimates of biodegradability useful in chemical screening, including the likelihood of passing a ready biodegradability test plus the approximate time required for a compound to biodegrade in a stream. Biodegradation is the destruction of a compound by biota, typically microorganisms, in the environment. Primary biodegradation is a change in molecular structure, and ultimate biodegradation is the complete conversion of the molecule to CO2 and H20.

BIOWIN has 6 models. The linear and a non-linear regression models, called BIOWIN 1 and BIOWIN 2, are based on regressions against 36 preselected chemical substructures plus molecular weight of experimental biodegradation data for 295 chemicals. The models correctly classified 90% of the chemicals in their training set as rapidly or not rapidly *biodegradable*. BIOWIN 3 and BIOWIN 4 estimate the approximate time required for ultimate and primary biodegradation, respectively, of an organic compound in streams. They are based on regressions of biodegradability estimates from a survey of experts for a suite of 200 organic chemicals, against the same chemical substructures plus molecular weight. BIOWIN 5 and BIOWIN 6 estimate the probability of passing the OECD 301C ready biodegradability test (MITI-1 test). They are based on linear (BIOWIN 5) and nonlinear (BIOWIN6) regressions of data from the Japanese MITI database against a modified set of chemical substructures plus molecular weight. Results were slightly better for the nonlinear model.

The EPI Suite of models were developed by Syracuse Research Corporation. All six of the models were developed under contract to the U.S EPA, OPPT, in support of Section 5 of TSCA.

How are the model predictions useful in risk assessment?

Whether a substance is readily biodegradable (RB) or not readily biodegradable (NRB) may have significant economic and regulatory impact. For example, in the European Community (EC) it is an important factor in classification and labeling under the dangerous substances directive. In the US, it is one of a small number of environmental fate data requirements included in the voluntary High Production Volume Chemical (HPVC) Challenge program. Applications in design and formulation of safer chemical products ("green chemistry") are also numerous because ready biodegradability is a useful basis for comparing alternatives. Recent work has demonstrated that model "batteries" consisting of BIOWIN3 and either BIOWIN5 or BIOWIN6 can be quite successful in classifying compounds as readily or not readily biodegradable; i.e. false positives for ready biodegradability are significantly reduced in number as compared to any individual model.

Knowing the time approximate required for a chemical to be broken down will help the risk assessor estimate the likely concentration of the chemical at various downstream locations and times after release to surface water. BIOWIN3 provides this information, which can be used in a variety of ways including serving as the basis for half-lives needed for running other models such as the PBT Profiler.

Chemicals with very long biodegradation times may be highly persistent in the environment IF they are not subject to destruction by other processes such as photolysis, hydrolysis, etc.

Formal pass criteria for OECD ready biodegradability tests:

>60 % of theoretical CO_2 evolution or biochemical oxygen demand in 28 days (>50% is also likely to be evidence of complete degradation of a compound, though this value is not formally recognized by the OECD)

>70% loss of dissolved organic carbon (DOC) derived from test compound.

General guidance for characterizing biodegradation rates:

Rapid	≥ 60% in	≤ 7 days
Moderate	≥ 30% in	≤ 28 days
Slow	< 30% in	≤ 28 days
Very slow	< 30% in	> 28 days

Examples of Biodegradation Values

CAS Number	Chemical	Ultimate Biodeg.
60571	Dieldrin	recalcitrant
1912249	Atrazine	months
75092	Dichloromethane	weeks-months
67641	Acetone	weeks
67561	Methanol	days-weeks

Inputs

CAS Registry Number or chemical structure in SMILES notation. When running models in the EPI Suite, available measured data should be entered because this will give more reliable estimates. This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

❖Molecular weight and formula
❖Predicted primary and ultimate biodegradation in hours, days, weeks, or months; also predicted, via separate but linked models, the probability of rapid biodegradation using two different methods; also predicted, via separate but linked models, the probability of passing a MITI-I (OECD 301C) ready biodegradability test
❖Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Where Can I Get BIOWIN™?

BIOWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run BIOWIN™ as a stand-alone model by putting a shortcut to the BIOWINNT.exe file on your Windows Desktop.

Saving Output

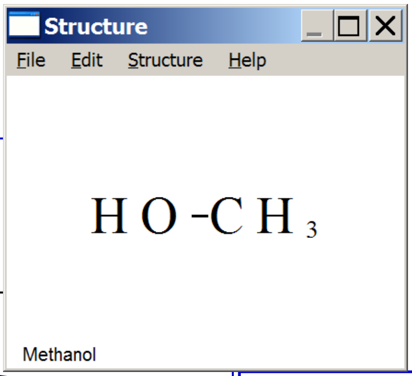
Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

Important Notes

1. Remember that BIOWIN can be run using SMILES notations instead of CAS numbers.
2. If your chemical is not in the SMILECAS database, you will need to write the SMILES and run the model using SMILES.
3. BIOWIN can be run as a part of the EPI Suite.
4. Biodegradation Probability > 0.5 from BIOWIN1 or 2 indicates "rapid biodegradation"; for BIOWIN5 or 6, indicates | Readily Degradable.
5. Biodegradation Probability < 0.5 from BIOWIN1 or 2 indicates "not rapid biodegradation"; for BIOWIN5 or 6, indicates | NOT Readily Degradable.
6. Biodegradation of "weeks" or faster from BIOWIN3 in combination with biodegradation probability > 0.5 from BIOWIN5 (or BIOWIN6) is even more reliable in indicating | Readily Degradable
7. When running models in the EPI Suite, available measured data should be entered because this will give more reliable estimates.

BIOWIN™ to Estimate Biodegradation

Sample Output from the BIOWIN™ Model



INPUTS: CAS Number = 67561 (methanol)
RESULTS:

```
SMILES    :  OC
CHEM      :  Methanol
MOL FOR   :  C1 H4 O1
MOL WT    :  32.04
-------------------------- BIOWIN v4.00 Results --------------------------
    Linear Model Prediction     :  Biodegrades Fast
    Non-Linear Model Prediction:  Biodegrades Fast
    Ultimate Biodegradation Timeframe:  Days-Weeks
    Primary  Biodegradation Timeframe:  Days
    MITI Linear Model Prediction     :  Readily Degradable
    MITI Non-Linear Model Prediction:  Readily Degradable
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                  | 0.1587  |  0.1587
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.0153
 Const|  *  |  Equation Constant                         |         |  0.7475
============+============================================+=========+=========
   RESULT   |     LINEAR BIODEGRADATION PROBABILITY      |         |  0.8910
============+============================================+=========+=========
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                  | 1.1178  |  1.1178
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.4550
============+============================================+=========+=========
   RESULT   |   NON-LINEAR BIODEGRADATION PROBABILITY    |         |  0.9752
============+============================================+=========+=========
 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                  | 0.1600  |  0.1600
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.0708
 Const|  *  |  Equation Constant                         |         |  3.1992
============+============================================+=========+=========
   RESULT   |   SURVEY MODEL - ULTIMATE BIODEGRADATION   |         |  3.2883
============+============================================+=========+=========
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                  | 0.1294  |  0.1294
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.0462
 Const|  *  |  Equation Constant                         |         |  3.8477
============+============================================+=========+=========
   RESULT   |   SURVEY MODEL - PRIMARY BIODEGRADATION    |         |  3.9310
============+============================================+=========+=========
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                  | 0.1611  |  0.1611
 Frag |  1  |  Methyl  [-CH3]                            | 0.0004  |  0.0004
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.0953
 Const|  *  |  Equation Constant                         |         |  0.7121
============+============================================+=========+=========
   RESULT   |  MITI LINEAR BIODEGRADATION PROBABILITY    |         |  0.7784
============+============================================+=========+=========
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                  | 1.0041  |  1.0041
 Frag |  1  |  Methyl  [-CH3]                            | 0.0194  |  0.0194
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.9250
============+============================================+=========+=========
   RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |         |  0.9324
============+============================================+=========+=========
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable
```

This chemical is predicted to biodegrade completely in days to weeks.

The 6 Models in BIOWIN are:

BIOWIN 1

BIOWIN 2

BIOWIN 3

BIOWIN 4

BIOWIN 5

BIOWIN 6

BCFWIN™ to Estimate Bioconcentration Factor

What Does the BCFWIN™ Model Do?

BCFWIN™ calculates the **B**io**C**oncentration **F**actor and its logarithm from the log KOW. The methodology is analogous to that for WSKOWWIN. Both are based on log Kow and correction factors. A bioconcentration factor (BCF) is the ratio (in L/kg) of a chemical's concentration in the tissue of an aquatic organism to its concentration in the ambient water, when exposure of the organism is to waterborne chemicals only (I.e., not to chemical in the organism's diet or sorbed to ingested particles).

The EPI Suite of models were developed by Syracuse Research Corporation. The BCFWIN Model was developed under contract to the U.S. EPA, OPPT, in support of Section 5 of TSCA.

How are the model predictions useful in risk assessment?

Knowing the fish BCF helps the risk assessor predict the potential for a chemicals to bioaccumulate in lipids (fatty tissue) of aquatic organisms.

Bioconcentration Potential	
High	≥ 5,000
Moderate	1,000 – 5,000
Low	< 1,000

Relationship Between log KOW and Fish BCF

As log KOW increases the solubility in lipids increases. This generally means an increase in the potential to bioconcentrate in aquatic organisms. This relationship begins to change around log KOW of 6. Above this value the situation is more complex because low water solubility limits the rate of uptake by the exposed organism. This means equilibrium may take a very long time to be achieved in bioconcentration studies, possibly too long to be practical. A result is that published data on BCF seem to show that BCF drops with increasing log KOW above log KOW of about 6. Some experts say that "true" bioconcentration potential continues to increase above log KOW ca. 6. Most likely, dietary exposure becomes dominant and exposure to waterborne chemical insignificant (remember– waterborne chemical only is a basic assumption for BCF to be valid!). What this really means is that **no simple "BCF/log KOW" relationship applies** at higher values of log KOW. That is, estimated BCF from BCFWIN is best used only below log KOW ca. 6.

Inputs

CAS Registry Number or chemical structure in SMILES notation. When running models in the EPI Suite, available measured data should be entered because this will give more reliable estimates. This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs

❖Molecular weight and formula
❖Estimated Log BCF
❖Estimated log KOW

Examples of Bioconcentration Factor Values

CAS Number	Chemical	Log BCF
8001352	Toxaphene	4.5
12789036	Chlordane	4.8
60571	Dieldrin	3.7
108703	1,3,5-Trichlorobenzene	2.7

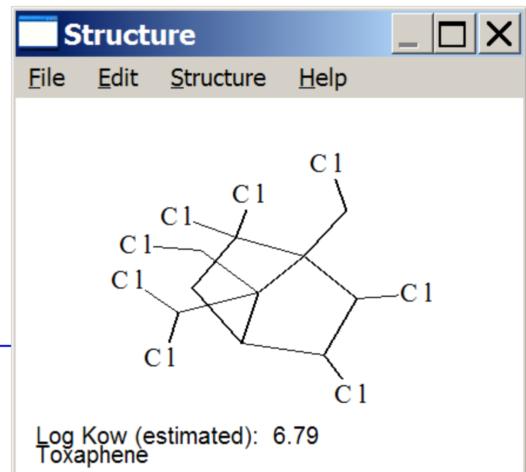
Where Can I Get BCFWIN™?

BCFWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/EPI Suitedl.htm. If you download and install EPI Suite™ you can run BCFWIN™ as a stand-alone model by putting a shortcut to the BCFWINNT.exe file on your Windows Desktop.

Saving Output

Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

Sample Output From the BCFWIN™ Model



INPUTS: CAS Number 8001352
(toxaphene)

RESULTS:

```
           Log BCF (v2.14 estimate): 3.75

SMILES : CLC(C(CL)C1C2)C(C2(CL)CL)(C1(C(CL)CL)CCL)CCL
CHEM   : Toxaphene
MOL FOR: C10 H10 CL8
MOL WT : 413.82
------------------ Bcfwin v2.14 ---------------------
Log Kow  (estimated)   :  6.79
Log Kow (experimental):  5.78
Log Kow used by BCF estimates:  5.78

Equation Used to Make BCF estimate:
   Log BCF = 0.77 log Kow - 0.70 + Correction

      Correction(s):                    Value
       No Applicable Correction Factors

   Estimated Log BCF =  3.751  (BCF = 5631)
```

STPWIN™ to Estimate Percent Removal in Wastewater Treatment

What Does the STPWIN™ Model Do?
STPWIN™ predicts the percent of a compound that will be removed from the waste water in wastewater treatment. Values are given for the total removal and three contributing processes (biodegradation, sorption to sludge, and stripping to air) for a standard system and set of operating conditions. STP is "Sewage Treatment Plant" and POTW is "Publicly Owned Treatment Works". Both are names for utilities that treat waste water and usually discharge the treated water to nearby surface water bodies.

How are the model predictions useful in a risk assessment?
Knowing how much of the chemical will be removed from the waste water during wastewater treatment enables the risk assessor to predict how much of the chemical may be discharged by the POTW to surface water and potentially affect aquatic life. How much chemical is discharged to surface water may also affect subsequant uptake by humans via drinking water that is derived from surface water.

Inputs
Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a "Batch Mode" so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measure data should be entered as well.

Outputs
❖Estimated percent removal in wastewater treatment
❖Overall chemical mass balance

Examples of Removal Rate Values

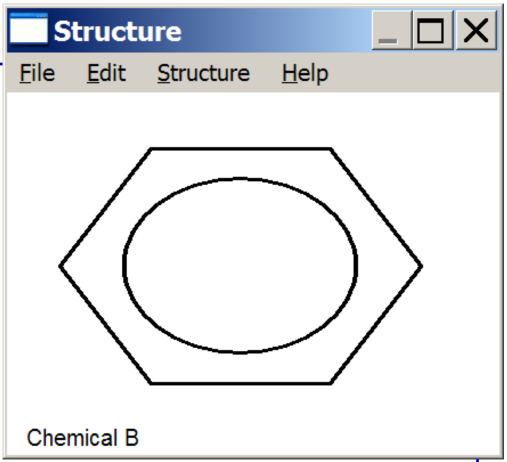
CAS Number	Chemical	Percent Removal
60571	Dieldrin	83.11
75092	Dichloromethane	56.91
50000	Formaldehyde	67.3
67641	Acetone	73.06
108952	Phenol	97.47

Where Can I Get STPWIN™?
STPWIN™ has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm.

Saving Output
Results can be printed when displayed. After results are displayed click on "Save Results" and you can save results as a ".dat" file that can be opened using MSWord or WordPerfect. Output can also be copied (click on "Copy") through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard. Further explanations are given in "Help" on the Results page.

STPWIN™ to Estimate Percent Removal in Wastewater Treatment

Sample Output From the STPWIN™ Model



INPUTS: SMILES : c1ccccc1
RESULTS:

```
SMILES :    c1ccccc1
CHEM   :    Chemical B
MOL FOR:    C6 H6
MOL WT :    78.11
    Physical Property Inputs:
    Water Solubility (mg/L):       1800
    Vapor Pressure (mm Hg) :       95.3
    Henry LC (atm-m3/mole) :      ------
    Log Kow (octanol-water):       ------
    Boiling Point (deg C)  :       ------
    Melting Point (deg C)  :       ------

STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
==========================================================================
PROPERTIES OF: Chemical B
-------------
Molecular weight (g/mol)    78.11
Aqueous solubility (mg/l)   1800
Vapour pressure (Pa)        12705.6
                (atm)       0.125395
                (mm Hg)     95.3
Henry 's law constant (Atm-m3/mol)          0.00555
Air-water partition coefficient             0.226978
Octanol-water partition coefficient (Kow)   134.896
Log Kow                                     2.13
Biomass to water partition coefficient      27.7793
Temperature [deg C]                         25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
  -Primary tank          0.00       526.34                   10000.00
  -Aeration tank         0.00       526.34                   10000.00
  -Settling tank         0.00       526.34                   10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                                       g/h              mol/h        percent
Influent                            1.00E+001          1.3E-001       100.00

Primary sludge                      5.63E-002          7.2E-004         0.56
Waste sludge                        5.46E-002          7.0E-004         0.55
Primary volatilization              1.25E-001          1.6E-003         1.25
Settling volatilization             1.10E-001          1.4E-003         1.10
Aeration off gas                    6.54E+000          8.4E-002        65.43

Primary biodegradation              1.82E-003          2.3E-005         0.02
Settling biodegradation             1.76E-004          2.2E-006         0.00
Aeration biodegradation             2.35E-003          3.0E-005         0.02

Final water effluent                3.11E+000          4.0E-002        31.06

Total removal                       6.89E+000          8.8E-002        68.94
Total biodegradation                4.35E-003          5.6E-005         0.04
```

Predicted Removal Rate in Waste Water Treatment is 69%

LEV3EPI™ Model to Estimate Fugacity

What Does the LEV3EPI™ Model Do?

The LEV3EPI Fugacity model is based on the LEVEL III fugacity model, developed by Don Mackay of Canadian Environmental Modelling Centre, Trent University, Ontario, Canada. LEV3EPI is a non-equilibrium, steady-state multimedia fate model that provides screening level predictions of environmental partitioning (percent in each media) of chemicals between air, soil, sediment, and water under steady state conditions for a default model "environment"; various defaults can be changed by the user. A risk assessor can use this model to estimate where a chemical is most likely to reside once it has been released to the environment.

How are the model predictions useful in risk assessment?

If the risk assessor understands a chemicals potential environmental partitioning he/she can use this information to manage the release scenario to minimize detrimental impacts to human health and the environment.

Inputs

Chemical structure (entered as CAS RN and retrieved from the accompanying SMILECAS database; SMILES notation; or drawn and saved as MDL). This program can be operated in a “Batch Mode” so that many structures (as SMILES strings, CAS RNs, or MDL files) can be entered and run at one time. Available measured physical/chemical properties and environmental half-lives should be entered (If not available these properties will be estimated by EPISuite™ components.)

Outputs

- partition coefficients
- Z values
- fugacity of each medium
- intermedia transport rates and D values
- reaction and advection D values and loss rates
- residence times or persistences (overall, reaction, and advection)
- concentrations and amounts for each medium
- summary diagram
- charts of key results, "readme.txt" file with more detailed technical information in a zipped file.

Examples of Fugacity Values

CAS RN	Chemical	Persistence (hrs)
8001352	Toxaphene	4260
12789036	Chlordane	4730
60571	Dieldrin	3040
108703	1,3,5-Trichlorobenzene	791
108952	Phenol	290

Important Notes

Default emission rates are equal amounts (1,000 kg/hr) to air, soil, and water (direct discharges to sediment are unlikely). The model treats a generic environment of 100,000 square km with 10% water; 90% soil surface; water depth 20 m; soil depth 20 cm; sediment depth 5 cm; atmospheric height 1000 m. The LEV3EPI™ model provides a representative environment about the size of the state of Ohio. It is important to note, however, that the percent in each medium will change as a function of the size of the compartments chosen. Moreover, the results of this model are calculated at steady state; a condition that may not occur in the environment (on a global scale).

LEV3EPI™ Model to Estimate Fugacity

Where Can I Get the LEV3EPI™ Model?

The LEV3EPI Fugacity model has been incorporated into the EPI Suite™ which is available at www.epa.gov/opptintr/exposure/docs/episuitedl.htm. If you download and install EPI Suite™ you can run LEV3EPI™ as a stand-alone model by putting a shortcut to the LEV3NT.exe file on your Windows Desktop.

Saving Output

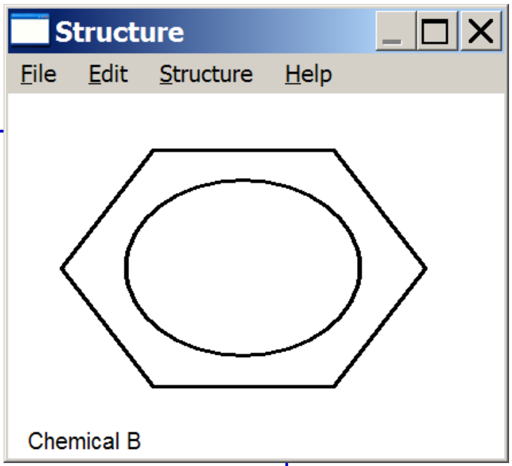
Results can be printed when displayed. After results are displayed click on “Save Results” and you can save results as a “.dat” file that can be opened using MSWord or WordPerfect. Output can also be copied (click on “Copy”) through the Windows Clipboard. Structures can be saved as an ISIS “.skc” file or through the Windows Clipboard. Further explanations are given in “Help” on the Results page.

Sample Output From the LEV3EPI™ Model

Run with default emission rates which assumes equal rates to Air, Water, Soil. Sediment is part of the water column.

Benzene (SMILES c1ccccc1)

	Percent in each media	Half-Life (hrs)
Air	38.0	209
Water	48.0	900
Soil	14.0	900
Sediment	0.2	0




```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name    : Chemical B
  Molecular Wt: 78.11
  Henry's LC   : 0.00555 atm-m3/mole (Henry database)
  Vapor Press  : 87.2 mm Hg  (MPBPVP™ program)
  Log Kow      : 2.13  (Kowwin program)
  Soil Koc     : 55.3  (calc by model)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)        (kg/hr)
   Air       37.6            209          1000
   Water     48.4            900          1000
   Soil      13.8            900          1000
   Sediment  0.202           3.6e+003     0

             Fugacity     Reaction     Advection    Reaction     Advection
              (atm)       (kg/hr)       (kg/hr)     (percent)    (percent)
   Air       5.91e-010     627          1.89e+003    20.9         62.9
   Water     8.65e-008     188          244          6.25         8.12
   Soil      1.64e-007     53.4         0            1.78         0
   Sediment  7.75e-008     0.196        0.0203       0.00652      0.000677

   Persistence Time: 168 hr
   Reaction Time:    579 hr
   Advection Time:   236 hr
   Percent Reacted:  28.9
   Percent Advected: 71.1

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      208.7
      Water:    900
      Soil:     900
      Sediment: 3600
        Biowin estimate: 2.441  (weeks-months)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```